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Calculation of a line list for manganese hydride (MnH) for brown dwarf and exoplanetary applications.

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Manganese Hydride in astronomy

To date, there are no astrophysical detections of MnH. However, as is pointed out by Halfen & Ziurys (2008), the cosmic abundance of manganese is of the same order as chromium: since chromium hydride (CrH) has found itself in a myriad of astronomical settings, it is quite possible that MnH could still be detected. The calculation of the line list presented in this poster hence opens up this possibility.

In addition to calculating a line list for the main isotopologue ^{55}MnH, line lists have been calculated for ^{53}MnH and ^{55}MnD. The ^{55}Mn isotopoe (stable) is of interest in supernova explosions (Iwamoto et al. 2009). Additionally Lugmair & Shukolyukov (1998) have investigated if the ^{53}Mn and ^{53}Cr isotopes can be used to determine timescales for solar system objects such as chondrites and meteorites. Also, since the possibility of using CrH and CrD spectra to infer the age of brown dwarfs has been postulated (Pavlenko et al. 2008) it was hence decided to generate linelists for the ^{55}MnD isotopologue.

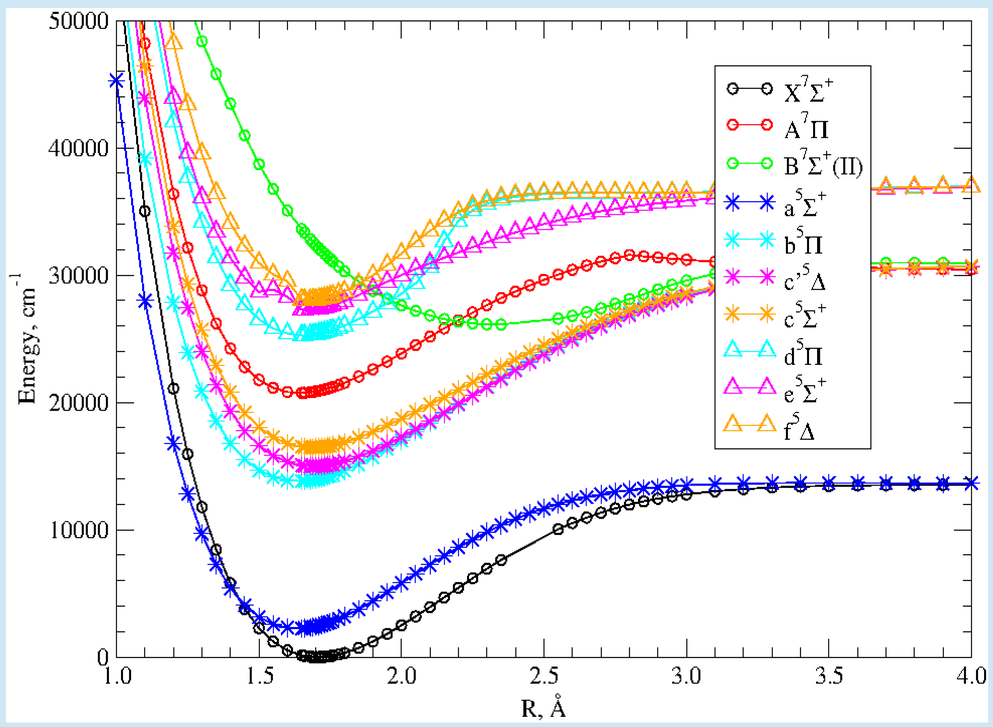

Fig 1. Ab initio Potential Energy Curves (PECs) used in the construction of the linelist for MnH. These PECs have been calculated using a cc-pVQZ/MRCI level of theory. Over 200 trial calculations were run in order to obtain these curves.

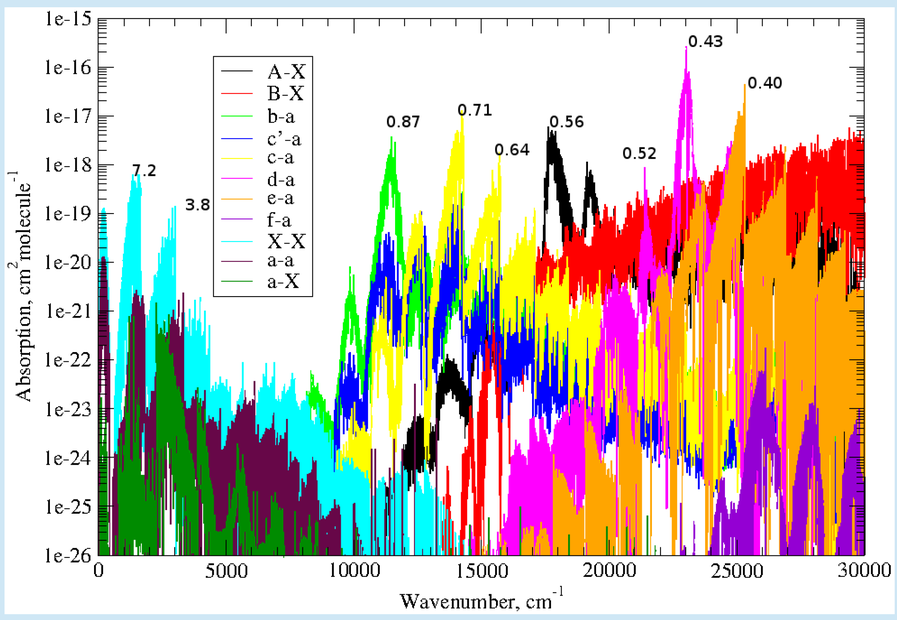

Fig 2. Cross-sectional absorption bands for the ^{55}MnH isotopomer calculated using a Gaussian profile with a half-width half-maximum of 1.0 at a temperature of 1500 K. The peaks have been annotated with values given in mircons. As can be seen many peaks lie within the visible region. MnH is an unusual transition-metal diatomic in that there is experimental data available for multiple electronic systems to which the line list has been refined to.

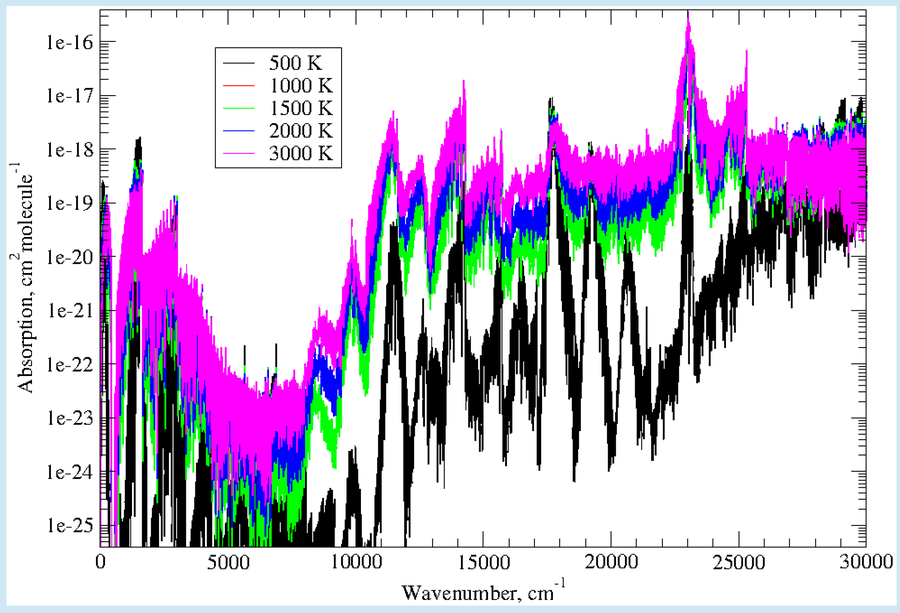

Fig 3. Effect of temperature on the absorption cross section for the $A^7\Pi$ – $X\ ^7\Sigma^+$ band of the ^{55}MnH isotopomer calculated using a Gaussian profile with a HWHM of 1.0.

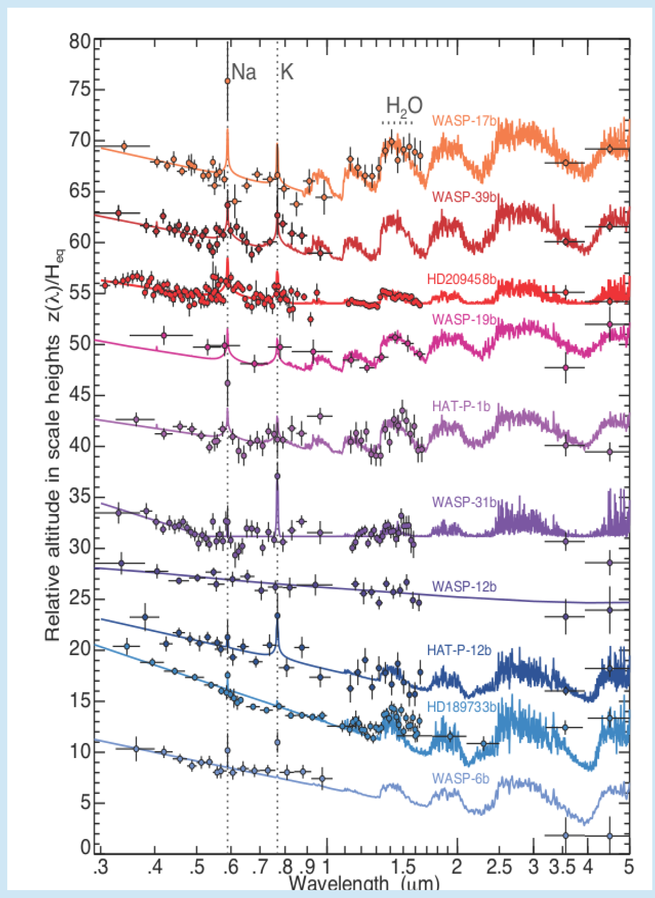

Fig 4. Figure taken from Sing et al. (2017) showing HST/Spitzer transmission spectral sequence of hot-Jupiter survey targets. This figure is included to show the comparison of the dominant emission regions of MnH compared to exoplanets.

Methodology

The calculation of line lists for transition metal containing (open d shells) diatomic molecules is a hugely challenging problem due to the myriad of low-lying coupled electronic states with high multiplicity (2S+1).

Following experience with calculating such a line list for CrH, a line list for the diatomic molecule of MnH has been calculated which encompasses the first low-lying bonding 10 electronic states.

A systematic series of high-level MRCI calculations was firstly undertaken (>200) in order to produce the most continuous and accurate *ab initio* curves.

Using experimental data available for both the septuplet and quinet electronic states, *ab initio* Potential Energy Curves (PECs) were then refined. For the $X\ ^7\Sigma^+$ and $A^7\Pi$ states, spectroscopic constants were taken from Gordon et al. (2005) and Gengeler et al. (2007) respectively and the program PGOPHER (Western 2010 & 2015) was used to convert these into a list of rovibronic energies. For the $a^5\Sigma^+$, $b^5\Pi$, $c^5\Sigma^+$, $d^5\Pi$ and $e^5\Sigma^+$ states, term values determined from Fourier Transform Spectrometer measurements from the work of Balfour et al. (1990, 1992) were used.

The program DUO which solves the coupled rovibronic Schrödinger equation was then used to calculate a refined line list which contains ~48 000 rovibronic states and ~5 million transitions. This line list includes states up to J = 50 and energy levels up to 32 000 cm^{-1} which should be adequate for temperatures up to 3000 K.

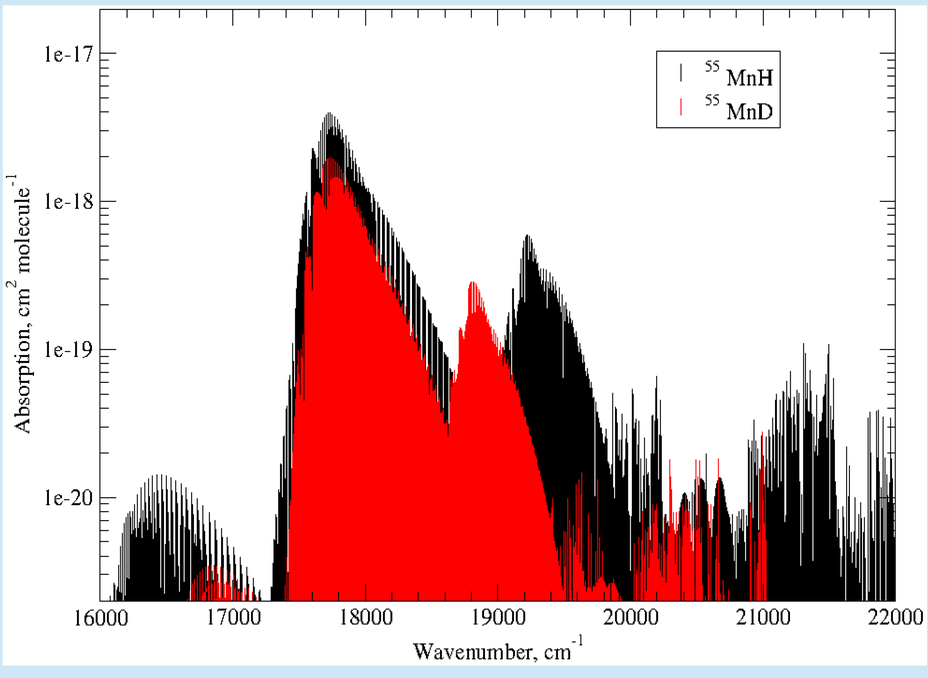

Fig 5. Comparison of the absorption band for the $A^7\Pi$ – $X\ ^7\Sigma^+$ band for ^{55}MnH and ^{55}MnD calculated using a Stick profile at a temperature of 1500 K. The diatomic molecule of CrH has been suggested as useful for the so-called “Deuterium test” (Pavlenko et al. 2007).

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